



WATER RESOURCES RESEARCH GRANT PROPOSAL

Project ID: WA1041

Title: Dye Tracers for Vadose Zone Hydrology

Focus Categories: Solute Transport, Hydrology

Keywords: Solute Transport, Groundwater Quality

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Congressional District: 5th

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Abstract

Hydrological research and hydrology in practice rely to a large degree on the use of tracers. Tracers are used to investigate flow pathways, to estimate travel and residence times, or to assess risks associated with pollution. Dyes are among the most prominent hydrological tracers, mainly due to their ease of detection, either visually by eye or analytically by spectrophotometry. Numerous dyes have been proposed as tracers, but no general recommendation for a suitable dye tracers can be made at this time. The dye tracer of choice depends on the purpose of the study as well as on the environmental conditions. The objective of the proposed research is to evaluate dyes in respect to their suitability as hydrological tracers. Specifically, we aim to establish correlations between the molecular structure of dye molecules and their environmental behavior, such as sorption and transport. Two classes of ionizable organic dyes will be chosen as model chemicals. In each class, a series of dyes with identical molecular backbone but different substituent groups will be selected. The sorption and transport of the dyes in soil and aquifer material will be evaluated with batch and column experiments. Quantitative structure activity relationships (QSAR) will be employed to analyze the experimental data. The molecular structure of the organic dyes will be characterized by molecular indices, such as the van der Waals volume and molecular connectivity. The relation between molecular indices and transport parameters will be analyzed by regression analysis. The proposed research will contribute to the identification of relevant mechanisms affecting transport of dyes in surface and subsurface waters. We will address the relation between molecular structure and transport properties in a systematic way, which enables us to make better predictions of fate and behavior of dye tracers in the aqueous environment. As a practical result of this project, we will be able to make scientifically sound and environmentally safe recommendations for the use of dye tracers for specific needs.